A Luttinger Liquid Coupled to a Quantum Spin Bath: Flow Equation Approach to the Kondo Necklace Model

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We study a lattice realization of a Luttinger liquid interacting with a bath of quantum spins in terms of an antiferromagnetic S=1/2 Heisenberg chain, where each spin is also coupled to a $\sigma = 1/2$ Kondo spin degree of freedom. This model describes the low-energy spin dynamics in quasi one dimensional materials, where the electronic spins of the magnetic ions interact with those of impurities, nuclei and possibly other spin species present in their environment. For large ferromagnetic and antiferromagnetic Kondo interaction J' there are two phases corresponding to an effective spin-1 Heisenberg chain and a dimerised spin-1/2 ladder, respectively. For weak Kondo interaction we establish that the Kondo interaction drives the system to a strong coupling regime. This suggests that $J' = 0$ is the only critical point in the system.

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I. INTRODUCTION

Entanglement and cooperative spin behaviour induced by coupling two spin systems with different intrinsic dynamics is a recurrent theme in condensed matter physics. In metals, it emerges in the context of the coupling between the spins of itinerant electrons and localized atomic/impurity spins, known as Anderson impurity or Kondo problem[1]. The famous "central spin" problem of an electronic system interacting with a bath of nuclear or impurity spins has recently re-emerged in the area of spin-polarized microelectronics and the physics of quantum, spin-entangled electronic states[2]. Perhaps the most interesting example of this kind is a quantum-critical spin system, such as found in strongly correlated magnetic insulators, coupled to a bath of quantum or classical spins[3,4,5,6,7,8,9]. In practice, the interaction between electronic spins in the system of interest and "external" spin variables arises in a variety of different contexts and occurs on vastly different energy scales. The first example is the exchange interaction between valence electrons involved in cohesion or chemical bonding and a localized "d"-orbital, such as in the s-d model of magnetic metals. If the d-orbital is singly occupied and the hybridization is weak, the dominant interaction is Kondo exchange[1]. Second is the coupling of electronic spins to impurity spins present in real material. While its effects scale with impurity concentration, in many cases and in particular at low temperatures it is the determining mechanism for physical phenomena such as damping and quantum decoherence. The response of a spin system that is either at or close to quantum criticality to impurity spins is particularly singular. It exhibits fascinating impurity-driven physics,[3,4], which has emerged in studies of lightly doped cuprates and related two-dimensional Mott insulators. Another example occurs in complex alloys, where in addition to magnetic $3d$ ions there often exist magnetic rare-earth cations (R^{3+}), which lead to a lattice of macroscopically many "impurity" spins even for ideal stoichiometric materials[5,6]. In the Haldane (S=1) chain atiferromagnet R_2BaNiO_5, the cooperative coupling to paramagnetic rare-earth spins dramatically modifies the spin dynamics of gapped Ni^{2+} chains and induces magnetic order at a finite temperature[6]. Finally, at very low energies/temperatures the hyperfine coupling of electronic and nuclear spins becomes important[7,8,9]. Indeed, many abundant isotopes of magnetic ions have non-zero nuclear spin[10]. Furthermore their electronic spins can also interact with nuclei of surrounding ligand ions[11].

Although in many cases the coupling of the spin system to external spin degrees of freedom can be neglected in the same way as the coupling to a generic thermostat is swept under the carpet in equilibrium statistical mechanics, it is of the same fundamental importance. The existence of such a coupling is required in order for the quantum (spin) system to reach its equilibrium state, or the ground state at T=0. Relaxation to equilibrium requires the change of both energy and angular momentum, which are integrals of motion for an isolated spin system. The simplest example is a Heisenberg magnet (or paramagnet) in a magnetic field. Here the Hamiltonian conserves the total spin component along the field direction. It is only through (the implicit) coupling to some external system of angular momenta, or spin bath, that the magnet can adjust its total spin as the magnetic field changes (e.g., in a quantum phase transition from a spin-gap to a magnetized phase).

While the effect of external spin degrees of freedom on the spin dynamics can often be averaged out, e.g., in the framework of spin-boson or spin-bath models[12,13], there are important cases where the coupled dynamics of the two systems is of paramount interest. One such case is

known as "pulling" – which refers to the hybrid dynamics in a system of electronic spins coupled to a thermalized ensemble of nuclear spins. Interest in this phenomenon was recently renewed by studies of field-induced quantum phase transitions in quantum magnets, where it was discovered that pulling prevents the expected full softening of the electronic spin excitation spectrum[14]. Instead, the latter acquires a gap, which increases with decreasing temperature, while a soft-mode behaviour is induced in the nuclear spins, which "take over" the quantum criticality[7,8,9].

Here we focus on the opposite, much less studied and understood limit of a quantum-critical spin system coupled to a bath of quantum spins, whose dynamics is governed solely by their Berry phases. We consider a Heisenberg S=1/2 chain with antiferromagnetic exchange coupling $J > 0$, where each spin is coupled to an additional local Kondo spin $\sigma = 1/2$ by an exchange J′,

$$H = J \sum_{\langle ij \rangle}^{N} \mathbf{S}(i) \cdot \mathbf{S}(j) + J' \sum_{i=1}^{N} \mathbf{S}(i) \cdot \boldsymbol{\sigma}(i). \tag{1}$$

This model is sometimes referred to as incomplete ladder, or SU(2) Kondo-necklace model, Fig. 1. The model (1) is a one-dimensional (1D) analog of the incomplete bilayer, which recently received much attention in the context of the 2D cuprates[15]. The fundamental difference between the 1D and 2D Kondo necklaces is that in D=2 quantum criticality is achieved by tuning the coupling J′, while in D=1 the S=1/2 chain is a critical Luttinger liquid for J′ = 0. In what follows we allow the Kondo-coupling J' in (1) to the local spins to be either ferromagnetic or antiferromagnetic.

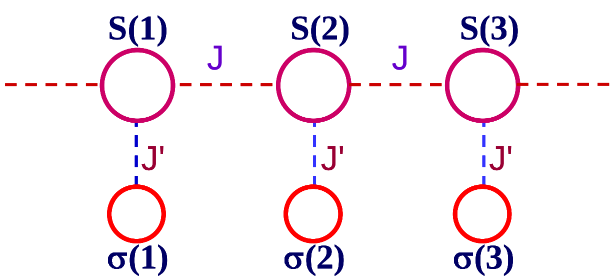

FIG. 1: One-dimensional Kondo necklace model: a "master" S = 1/2 Heisenberg chain with antiferromagnetic coupling J, where each spin interacts with an extra, Kondo spin degree of freedom $\sigma = 1/2$, via coupling J'.

The model (1) is closely related to the Kondo necklace model,

$$H_{\rm KNM} = J \sum_{\langle ij \rangle}^{N} S^x(i)S^x(j) + S^y(i)S^y(j) + J' \sum_{i=1}^{N} \mathbf{S}(i) \cdot \boldsymbol{\sigma}(i), \tag{2}$$

which was introduced in Ref. 16 as a simplified version of the Kondo lattice model in the 1D case. The Kondo necklace model (2) has been studied by a variety of methods such as Monte Carlo simulations[17], real-space renormalization group (RG) techniques[18], exact numerical diagonalization[19], density-matrix renormalization group (DMRG) computations[20,21], bond operator mean field theory[22,23] and bosonization[24,25]. While all methods agree in the regime $|J'| \gg J$, it is still controversial whether a small Kondo coupling $|J'| \ll J$ leads to the formation of a spin gap. While real-space RG and exact diagonalization of small systems suggest the existence of a critical value J'_c of the Kondo coupling strength, below which the spin gap vanishes, Monte-Carlo and DMRG computations indicate that in fact $J'_c = 0$. The doped case has recently been investigated in[26]. In the two and three-dimensional cases it is well established that there is a quantum phase transition between a Néel ordered ground state at small $J' > 0$ and a Kondo-singlet phase at $J' > J'_c$[22,23,27,28,29].

In the present work we study the model (1) using the flow equation method. In order to "close" the system of flow equations we employ a decoupling scheme for spin operator products, which is asymptotically valid in the limit $J' \to 0$, and use essentially exact expressions for the two-spin correlation function in the "master" spin-1/2 chain, derived by field theory methods[30,31]. The flow equations obtained upon decoupling are then solved numerically in the weak coupling limit.

II. STRONG COUPLING LIMITS

In order to understand general properties and phase diagram of the model, it is instructive to analyze the strong coupling limits $J' \to \pm\infty$ first.

A. Ferromagnetic Kondo coupling $J' \to -\infty$

For strong ferromagnetic Kondo coupling an effective spin 1 is formed on each rung. The Hamiltonian describing the interaction between these spins takes the form of an antiferromagnetic spin-1 Heisenberg chain

$$H_{\rm eff} = \frac{J}{4} \sum_j \vec{T}_j \cdot \vec{T}_{j+1}. \tag{3}$$

Here T_j^α are spin-1 operators. The antiferromagnetic spin-1 chain is known to display a spontaneously broken $Z_2 \otimes Z_2$ symmetry characterized by a non-zero string order $\mathcal{O}^\alpha_{\rm string} \neq 0$, where[32]

$$\mathcal{O}^\alpha_{\rm string} = \lim_{n\to\infty} \left\langle T^\alpha_j \exp\Big(i\pi \sum_{k=j+1}^{j+n-1} T^\alpha_k\Big) T^\alpha_{j+n} \right\rangle. \tag{4}$$

It is well known that excitations in the spin-1 Heisenberg chain are desribed in terms of a triplet of gapped magnons.

B. Antiferromagnetic Kondo coupling $J' \to \infty$

In this limit the ground state is that of decoupled singlet dimers. This is in fact the same ground state as for the regular two-leg ladder with $J_{\rm rung} \gg J_{\rm leg}$ in the limit $J_{\rm rung} \to \infty$. It also can be characterized by a string order parameter, e.g.,[33]

$$\begin{aligned} \mathcal{O}_{\rm string} &= \lim_{n\to\infty} \left\langle \prod_{k=j}^{j+n} \left[-4\sigma_j^z S_j^z\right] \right\rangle \\ &= \lim_{n\to\infty} \left\langle \exp\Big(i\pi \sum_{k=j}^{j+n} \sigma_k^z + S_k^z \Big) \right\rangle . \end{aligned} \tag{5}$$

The excitation spectrum in this limit again has a gap.

III. WEAK KONDO COUPLING

The question we want to address is what happens for weak Kondo couplings $|J'| \ll J$. The Kondo necklace model can be viewed as a particular limit of an asymmetric two-leg ladder model, in which the coupling along the first leg J is much larger than the rung coupling J', which in turn is large compared to the exchange J_2 along the second leg

$$J \gg J' \gg J_2. \tag{6}$$

This case is difficult to analyze for the following reason. Bosonizing the spin chains making up the two legs of the ladder results in a two-flavour Luttinger liquid. However, the cutoff of this theory is equal to J_2. The rung coupling J' can then not be treated as a perturbation of the two-flavour Luttinger liquid as it is much larger than the cutoff of the latter. In the Kondo necklace model the role of J_2 is played by the RKKY interaction induced by J', which is of order $J'^2/J \ll |J'|$.

In order to analyze the small J' regime we have employed Wegner's flow equation method[34,35,36,37,38,39].

A. Flow Equation Method

In the flow equation method[34,35] a one-parameter family of unitarily equivalent Hamiltonians $H(l)$ is constructed via the differential equation

$$\frac{dH(l)}{dl} = [\eta(l), H(l)]. \tag{7}$$

The anti-hermitian generator $\eta(l)$ is taken as

$$\eta(l) = [H_0(l), H(l)], \tag{8}$$

where $H_0(l)$ is a particularly chosen "diagonal" part of the Hamiltonian. For the Kondo necklace model we chose $H_0(l)$ as

$$\begin{aligned} H_0(l) &= \frac{1}{N}\sum_k J_k(l)\ \mathbf{S}_k\cdot\mathbf{S}_{-k} \\ &+ \frac{1}{N}\sum_k \alpha_k(l)\ \boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_{-k}. \end{aligned} \tag{9}$$

Here the Fourier transformed spin operators are defined as

$$\mathbf{S}_k = \sum_n \mathbf{S}(n) e^{-ikn}, \quad \mathbf{S}(n) = \frac{1}{N}\sum_k \mathbf{S}_k e^{ikn}. \tag{10}$$

In the initial Hamiltonian (1) the second term is absent, but it will be generated under the flow. The full Hamiltonian will be of the form

$$H(l) = H_0(l) + H_1(l) + H_2(l)\ , \tag{11}$$

where

$$H_1(l) = \frac{1}{N}\sum_k J'_k(l) \mathbf{S}_k\cdot\boldsymbol{\sigma}_{-k}\ . \tag{12}$$

The contribution $H_2(l)$ will loosely speaking contain all multi-spin interaction terms compatible with the global SU(2) spin rotational symmetry. A key element in implementing the flow equation approach is that the initial coupling J' is small and all terms in $H_2(l)$ will be of order J'^2 or higher. As long as we constrain our attention to the small J' limit, we may therefore neglect $H_2(l)$ when calculating the generator $\eta(l)$ of the unitary transformation

$$\eta(l) = [H_0(l), H_1(l)] = \eta_1(l) + \eta_2(l). \tag{13}$$

The explicit forms of $\eta_{1,2}(l)$ are

$$\begin{aligned} \eta_1(l) &= \frac{i}{N^2}\sum_{kk'} J'_{k'}(l)[J_k(l) - J_{k+k'}(l)] \\ &\qquad [\mathbf{S}_{k+k'}\times\mathbf{S}_{-k}]\cdot\boldsymbol{\sigma}_{-k'}, \\ \eta_2(l) &= \frac{i}{N^2}\sum_{kk'} J'_{k'}(l)[\alpha_k(l) - \alpha_{k+k'}(l)] \\ &\qquad [\boldsymbol{\sigma}_{k+k'}\times\boldsymbol{\sigma}_{-k}]\cdot\mathbf{S}_{-k'}. \end{aligned} \tag{14}$$

Working out the required commutators of $\eta_{1,2}(l)$ with $H_{0,1}(l)$ (see Appendix A) we arrive at the following ex-

pression for the Hamiltonian $H(l)$

$$\begin{aligned} H(l) &= \frac{1}{N}\sum_k J_k(l)\mathbf{S}_k\cdot\mathbf{S}_{-k} + \frac{1}{N}\sum_k \alpha_k(l)\boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_{-k} \\ &+ \frac{1}{N}\sum_k J'_k(l)\mathbf{S}_k\cdot\boldsymbol{\sigma}_{-k} \\ &+ \frac{1}{N^3}\sum_{k,p,q} M^{(1)}_{k,p,q}(l)\ \mathbf{S}_{k+p+q}\cdot\boldsymbol{\sigma}_{-p}\ \mathbf{S}_{-k}\cdot\boldsymbol{\sigma}_{-q} \\ &+ \frac{1}{N^3}\sum_{k,p,q} M^{(2)}_{k,p,q}(l)\ \mathbf{S}_{k+p}\cdot\mathbf{S}_{q}\ \mathbf{S}_{-k}\cdot\boldsymbol{\sigma}_{-p-q} \\ &+ \frac{1}{N^3}\sum_{k,p,q} M^{(3)}_{k,p,q}(l)\ \mathbf{S}_{k+p+q}\cdot\mathbf{S}_{-k}\ \boldsymbol{\sigma}_{-q}\cdot\boldsymbol{\sigma}_{-p} \\ &+ \frac{1}{N^3}\sum_{k,p,q} M^{(4)}_{k,p,q}(l)\ \boldsymbol{\sigma}_{k+p}\cdot\boldsymbol{\sigma}_{q}\ \boldsymbol{\sigma}_{-k}\cdot\mathbf{S}_{-p-q} \\ &+ \frac{i}{N^3}\sum_{k,p,q} M^{(5)}_{k,p,q}(l)\ [\mathbf{S}_{k+p+q}\times\mathbf{S}_{-k}]\cdot\boldsymbol{\sigma}_{-p-q} \\ &+ \frac{i}{N^3}\sum_{k,p,q} M^{(6)}_{k,p,q}(l)\ [\boldsymbol{\sigma}_{k+p+q}\times\boldsymbol{\sigma}_{-k}]\cdot\mathbf{S}_{-p-q}. \end{aligned} \tag{15}$$

The initial values of the various couplings are

$$J_k(0) = J\cos k,\quad J'_k(0) = J',\quad M^{(a)}_{k,p,q}(0) = 0.$$

In order to obtain a set of flow equations we need to decouple the three- and four-spin terms. We do this by expanding in fluctuations around the $J'=0$ ground state, i.e.,

$$\begin{aligned} \mathbf{S}_k\cdot\mathbf{S}_{k'}\ \boldsymbol{\sigma}_q\cdot\boldsymbol{\sigma}_{-k-k'-q} &= \langle\mathbf{S}_k\cdot\mathbf{S}_{k'}\rangle\boldsymbol{\sigma}_q\cdot\boldsymbol{\sigma}_{-k-k'-q} \\ &+\langle\boldsymbol{\sigma}_q\cdot\boldsymbol{\sigma}_{-k-k'-q}\rangle\mathbf{S}_k\cdot\mathbf{S}_{k'} \\ &+ :\mathbf{S}_k\cdot\mathbf{S}_{k'}\ \boldsymbol{\sigma}_q\cdot\boldsymbol{\sigma}_{-k-k'-q}:, \end{aligned} \tag{16}$$

$$\begin{aligned} \mathbf{S}_{k'}\cdot\boldsymbol{\sigma}_q\ \mathbf{S}_k\cdot\boldsymbol{\sigma}_{-k-k'-q} &= \frac{1}{3}\langle\mathbf{S}_{k'}\cdot\mathbf{S}_{k}\rangle\boldsymbol{\sigma}_q\cdot\boldsymbol{\sigma}_{-k-k'-q} \\ &+\frac{1}{3}\langle\boldsymbol{\sigma}_q\cdot\boldsymbol{\sigma}_{-k-k'-q}\rangle\mathbf{S}_{k'}\cdot\mathbf{S}_{k} \\ &+ :\mathbf{S}_{k'}\cdot\boldsymbol{\sigma}_q\ \mathbf{S}_k\cdot\boldsymbol{\sigma}_{-k-k'-q}:, \end{aligned} \tag{17}$$

$$\begin{aligned} \mathbf{S}_k\cdot\mathbf{S}_{k'}\ \mathbf{S}_q\cdot\boldsymbol{\sigma}_{-k-k'-q} &= \langle\mathbf{S}_k\cdot\mathbf{S}_{k'}\rangle\mathbf{S}_q\cdot\boldsymbol{\sigma}_{-k-k'-q} \\ &+\frac{1}{3}\langle\mathbf{S}_k\cdot\mathbf{S}_{q}\rangle\mathbf{S}_{k'}\cdot\boldsymbol{\sigma}_{-k-k'-q} \\ &+\frac{1}{3}\langle\mathbf{S}_{k'}\cdot\mathbf{S}_{q}\rangle\mathbf{S}_{k}\cdot\boldsymbol{\sigma}_{-k-k'-q} \\ &+ :\mathbf{S}_k\cdot\mathbf{S}_{k'}\ \mathbf{S}_q\cdot\boldsymbol{\sigma}_{-k-k'-q}:\ . \end{aligned} \tag{18}$$

These expansions can be motivated by bosonizing the Hamiltonian (15) (see Appendix B). Substituting (18) into (15) we obtain expressions for $H_0(l)$ and $H_1(l)$. The static spin-spin correlation functions entering (18) and hence the expressions for $H_{0,1}(l)$ should be calculated self-consistently with respect to the flowing Hamiltonian $H_0(l)$. However, at weak coupling $|J'| \ll J$ one may calculate the correlators with respect to the initial Hamiltonian $H_0(0)$, as the corrections are of higher order in J'. Taking into account that

$$\begin{aligned} \langle\mathbf{S}_k\cdot\mathbf{S}_{k'}\rangle &= \delta_{k,-k'}\langle\mathbf{S}_k\cdot\mathbf{S}_{-k}\rangle\ , \\ \langle\boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_{k'}\rangle &= \frac{3N}{4}\delta_{k,-k'}\ , \end{aligned} \tag{19}$$

and retaining only terms quadratic in spin operators, the Hamiltonian (15) is reduced to

$$\begin{aligned} \tilde{H}(l) &= \frac{1}{N}\sum_k J_k(l)\ \mathbf{S}_k\cdot\mathbf{S}_{-k} + \frac{1}{N}\sum_k \alpha_k(l)\ \boldsymbol{\sigma}_k\cdot\boldsymbol{\sigma}_{-k} \\ &+\frac{1}{N}\sum_k J'_k(l)\ \mathbf{S}_k\cdot\boldsymbol{\sigma}_{-k}. \end{aligned} \tag{20}$$

The flow equations for the couplings take the form

$$\frac{dJ_k}{dl} = \frac{2}{3N}\sum_{k'}(J'_{k'})^2(2J_k - J_{k+k'} - J_{k-k'})\frac{\langle\boldsymbol{\sigma}_{k'}\cdot\boldsymbol{\sigma}_{-k'}\rangle}{N} + \frac{2(J'_k)^2}{3N}\sum_{k'}(2\alpha_{k'} - \alpha_{k+k'} - \alpha_{k-k'})\frac{\langle\boldsymbol{\sigma}_{k'}\cdot\boldsymbol{\sigma}_{-k'}\rangle}{N}, \tag{21}$$

$$\frac{d\alpha_k}{dl} = \frac{2}{3N}\sum_{k'}(J'_{k'})^2(2\alpha_k - \alpha_{k+k'} - \alpha_{k-k'})\frac{\langle\mathbf{S}_{k'}\cdot\mathbf{S}_{-k'}\rangle}{N} + \frac{2(J'_k)^2}{3N}\sum_{k'}(2J_{k'} - J_{k+k'} - J_{k-k'})\frac{\langle\mathbf{S}_{k'}\cdot\mathbf{S}_{-k'}\rangle}{N}, \tag{22}$$

$$\frac{dJ'_k}{dl} = \frac{4J'_k}{3N}\sum_{k'}\Big\{(J_{k'}-J_k)(J_{k+k'}+J_{k-k'}-2J_{k'})\frac{\langle \mathbf{S}_{k'}\cdot\mathbf{S}_{-k'}\rangle}{N} + (\alpha_{k'}-\alpha_k)(\alpha_{k+k'}+\alpha_{k-k'}-2\alpha_{k'})\frac{\langle \boldsymbol{\sigma}_{k'}\cdot\boldsymbol{\sigma}_{-k'}\rangle}{N}\Big\}$$
$$+\frac{4}{3N}\sum_{k'} J'_{k'}J'_{k+k'}\Big\{(J_{k+k'}-J_k)\frac{\langle \mathbf{S}_{k+k'}\cdot\mathbf{S}_{-k-k'}\rangle}{N} + (\alpha_{k+k'}-\alpha_k)\frac{\langle \boldsymbol{\sigma}_{k+k'}\cdot\boldsymbol{\sigma}_{-k-k'}\rangle}{N}\Big\}. \tag{23}$$

As we have remarked earlier, in order to solve the flow equations we need to know the static spin-spin correlator $\langle \mathbf{S}_k \cdot \mathbf{S}_{-k}\rangle$ for the isotropic spin-1/2 Heisenberg chain. This can be calculated accurately from the results of Refs. [30,31]. There the large distance asymptotics of spin-spin correlations functions was determined by combining exact results for correlation amplitudes[40] with renormalization group improved perturbation theory in the marginally irrelevant interaction of spin currents present in the continuum description of the spin-1/2 Heisenberg chain that

$$\langle \mathbf{S}(m+j)\cdot\mathbf{S}(j)\rangle \approx \frac{3}{4}\left[\frac{(-1)^m}{m}\sqrt{\frac{2}{\pi^3 g}}f_1(g) - \frac{f_2(g)}{\pi^2 m^2}\right], \tag{24}$$

where

$$\begin{aligned} f_1(g) &= 1+\Big(\frac{3}{8}-\frac{c}{2}\Big)g+\Big(\frac{5}{128}-\frac{c}{16}-\frac{c^2}{8}\Big)g^2 \\ &+ \Big(\frac{21}{1024}+\frac{7c}{256}-\frac{7c^2}{64}-\frac{c^3}{16}+\frac{13\,\zeta(3)}{32}\Big)g^3, \\ f_2(g) &= 1+\frac{g}{2}+\Big(c+\frac{3}{4}\Big)\frac{g^2}{2}+\frac{c(c+2)}{2}g^3. \end{aligned} \tag{25}$$

Here g is the running coupling constant

$$\sqrt{g}\ e^{1/g} = 2\sqrt{2\pi}\ e^{\gamma_E + c}\ m\ , \tag{26}$$

and c is a free parameter that related to the choice of renormalization scheme. It was demonstrated in Ref. [31] that for $l \geq 2$ (24) is in very good agreement with numerical results. Supplementing these results with the known values

$$\begin{aligned} \langle \mathbf{S}(j)\cdot\mathbf{S}(j+1)\rangle &= \frac{1}{4}+\sum_{n=1}^{\infty}\frac{(-1)^n}{n} = -0.443147...\ , \\ \langle \mathbf{S}(j)\cdot\mathbf{S}(j)\rangle &= \frac{3}{4}\ , \end{aligned} \tag{27}$$

and then Fourier transforming, we arrive at the result shown in Fig.2. We see that in momentum space the spin-spin correlator is dominated by the logarithmic divergence at $k=\pi$.

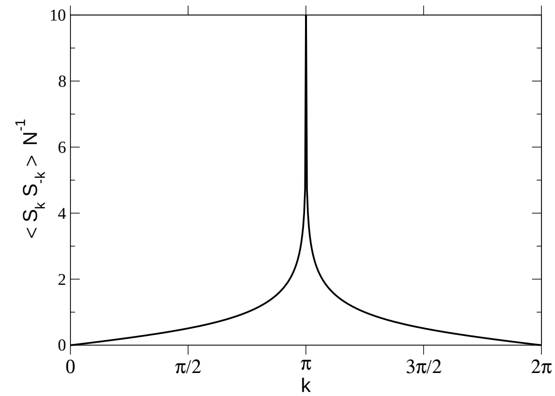

FIG. 2: Static spin-spin correlation function on the isotropic spin-1/2 Heisenberg chain.

B. Solution of the Flow Equations

We are now in a position to solve the flow equations (21)-(23) numerically. We find that for small initial values on the Kondo interaction $|J'| < 0.1J$ the behaviour of the solutions to the flow equations exhibits two regimes. In the following we measure l in units of J^{-2}. For large flow parameters $l \gtrsim 100$ the couplings appear to approach a fixed point. However, as l increases further, the behaviour eventually changes and the couplings diverge. We interpret the eventual runaway flow as being indicative of the emergence of a strong coupling phase, characterized by the formation of a spectral gap.

1. Kondo Interaction

We find that for $l \gtrsim 100$ and small initial values of the Kondo interaction $|J'| < 0.1J$, the couplings J'_k become very small everywhere except at $k = 0, 2\pi$. This holds in the ferromagnetic as well as the antiferromagnetic case. This behaviour is shown in Fig.3, where we plot J'_k as a function of k for different values of l and $J' = 0.05J$. The vicinity of $k = 2\pi$ is shown in greater detail in Fig.4.

In Fig.5 we show the Kondo coupling in the vicinity of $k=\pi$ for several values of the flow parameter l. We observe that for large values of l $J'_k(l)$ appears to approach a small but finite limit. In position space the Kondo coupling J' becomes more and more long-ranged as the flow parameter l increases. This is shown in Fig.6. For very large values of the flow parameter l we always enter a regime in which the J'_k diverge. This is shown for the case $J' = 0.06J$ in Fig.7.

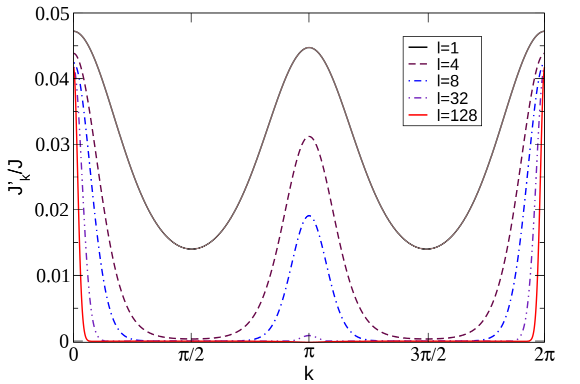

FIG. 3: Kondo coupling J'_k as a function of the momentum k for several values of the parameter l characterizing the flow $l = 1$, $l = 4$, $l = 8$, $l = 32$ and $l = 128$. The initial value is $J'_k = 0.05J$. The Kondo interaction becomes small under the flow except in the vicinity of $k = 0, 2\pi$.

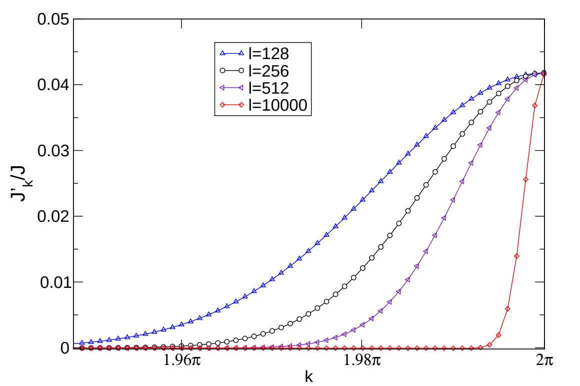

FIG. 4: Kondo coupling J'_k in the vicinity of $k = 2\pi$ for several values of the parameter l characterizing the flow. The initial value is $J'_k = 0.05J$.

2. RKKY Interaction

The flow of the RKKY couplings $\alpha_k(l)$ is shown in Fig.8 for several values of the flow parameter l. We see that the flow appears to approach a small finite limit quite quickly. The RKKY couplings are strongest in the vicinity of $k = \pi$, where they become of order J'^2/J.

For sufficiently large values of the flow parameter l the RKKY interaction starts to decrease quite quickly and eventually diverges.

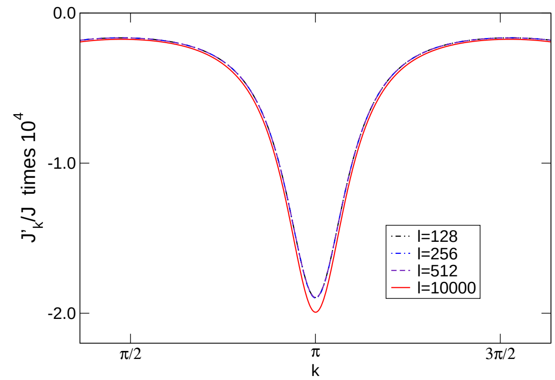

FIG. 5: Kondo coupling J'_k as a function of the momentum k in the vicinity of $k = \pi$ for several values of the parameter l characterizing the flow. The initial value is $J'_k = 0.05J$. The couplings J'_k tend to a small but finite limit for large values of l.

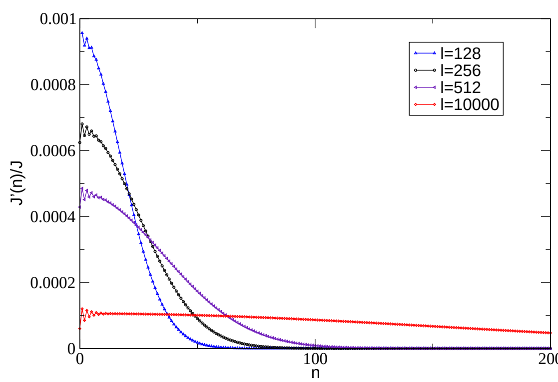

FIG. 6: Kondo coupling $J'(n)$ in coordinate space for valious values of the flow parameter l. The initial value of the Kondo coupling is $J' = 0.05J$. There is a long range smooth component as well as a shorter range staggered one.

3. Heisenberg Interaction

The Heisenberg interaction changes only weakly under the flow. We therefore plot the difference $J_k(l) - J_k(0)$ rather than $J_k(l)$ itself in Fig.9. We find that the k dependence is unchanged under the flow, so that

$$J_k(l) = J(l)\cos(k)\ . \tag{28}$$

Here $J(l) = J + \mathcal{O}\big(J'^2/J\big)$.

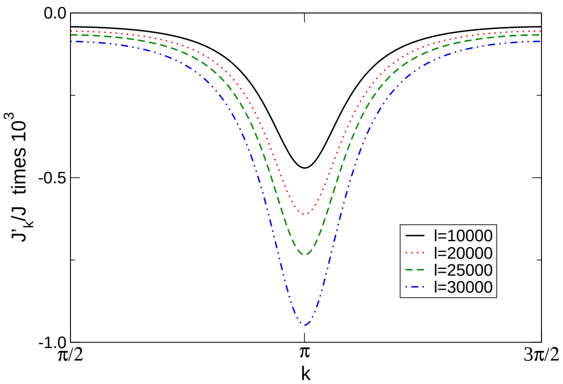

FIG. 7: Kondo coupling J_k' as a function of the momentum k in the vicinity of $k = \pi$ for large values of the parameter l characterizing the flow. The initial value is $J' = 0.06J$. The absolute values of the couplings are seen to increase with l.

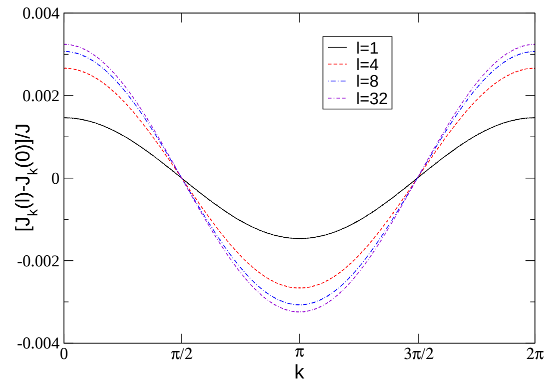

FIG. 9: Difference of Heisenberg couplings $J_k(l) - J_k(0)$ as a function of the momentum k for several values of the parameter l characterizing the flow $l = 1$, $l = 4$, $l = 8$, $l = 32$. The initial value was taken to be $J_k' = 0.05J$.

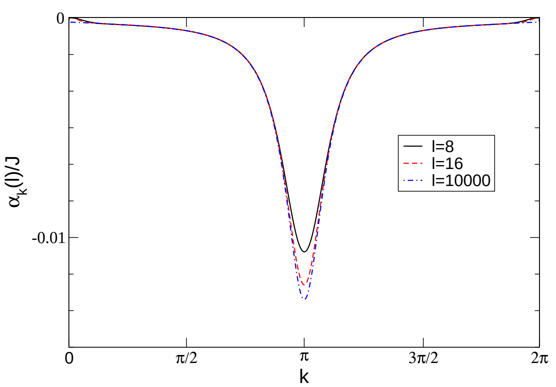

FIG. 8: RKKY coupling α_k as a function of the momentum k for several values of the parameter l characterizing the flow. The initial value is $J_k' = 0.05J$.

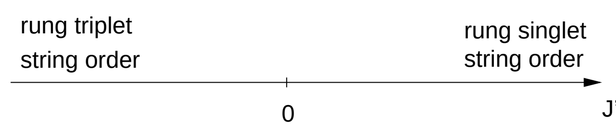

FIG. 10: Zero temperature phase diagram of the SU(2) invariant one dimensional Kondo necklace model.

IV. DISCUSSION

The above analysis of the flow equations shows that a small Kondo interaction drives the system to a strong coupling regime. On the basis of the analysis presented in this work we cannot establish the nature of the strong coupling phase. However, using exact diagonalization of small systems one can see that there is a spin gap for $J' \gtrsim 0.3J$, which suggests that the large-J' phase extends at least down to such interaction strengths. Combining this observation with the result of the flow equation analysis suggests a form of the phase diagram as shown in Fig.10. This would imply there presence of a spin gap Δ for any $J' \neq 0$, but the flow equation approach presented here does not allow for a determination of how Δ scales with J'.

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APPENDIX A: COMMUTATORS

In this appendix we list the commutators needed for determining the flow equations.

$$\begin{aligned}[\eta_1, H_0] &= \frac{1}{N^3}\sum_{k,p,q}\Gamma^{(1)}_{k,p,q}\,\mathbf{S}_{k+p}\times\mathbf{S}_{-k}\cdot\boldsymbol{\sigma}_{q-p}\times\boldsymbol{\sigma}_{-q}\\ &+\frac{1}{N^3}\sum_{k,p,q}\Gamma^{(2)}_{k,p,q}\mathbf{S}_q\cdot\mathbf{S}_{-k}\;\mathbf{S}_{k+p-q}\cdot\boldsymbol{\sigma}_{-p}.\end{aligned}\tag{A1}$$

$$[\eta_2, H_0] = \frac{1}{N^3}\sum_{k,p,q}\Gamma^{(3)}_{k,p,q}\boldsymbol{\sigma}_{k+p}\times\boldsymbol{\sigma}_{-k}\cdot\mathbf{S}_{q-p}\times\mathbf{S}_{-q} + \frac{1}{N^3}\sum_{k,p,q}\Gamma^{(4)}_{k,p,q}\boldsymbol{\sigma}_{q}\cdot\boldsymbol{\sigma}_{-k}\ \boldsymbol{\sigma}_{k+p-q}\cdot\mathbf{S}_{-p}. \quad (A2)$$

$$\begin{aligned}[\eta_1, H_1] = \frac{1}{N^3}\sum_{k,p,q}\Gamma^{(5)}_{k,p,q}\Big\{&\mathbf{S}_{k+p+q}\cdot\boldsymbol{\sigma}_{-p}\ \mathbf{S}_{-k}\cdot\boldsymbol{\sigma}_{-q}\\ &+\mathbf{S}_{k+p}\cdot\mathbf{S}_{q}\ \mathbf{S}_{-k}\cdot\boldsymbol{\sigma}_{-p-q}\\ &-\mathbf{S}_{k+p+q}\cdot\mathbf{S}_{-k}\ \boldsymbol{\sigma}_{-q}\cdot\boldsymbol{\sigma}_{-p}\\ &-i\left[\mathbf{S}_{k+p+q}\times\mathbf{S}_{-k}\right]\cdot\boldsymbol{\sigma}_{-p-q} + \text{h.c.}\Big\}. \quad (A3)\end{aligned}$$

$$\begin{aligned}\Gamma^{(1)}_{k,p,q} &= J'_p\left[J_k - J_{k+p}\right]\left[\alpha_q - \alpha_{p-q}\right],\\ \Gamma^{(2)}_{k,p,q} &= -4J'_p\left[J_k - J_{k+p}\right]\left[J_q - J_{k+p-q}\right],\\ \Gamma^{(3)}_{k,p,q} &= J'_p\left[\alpha_k - \alpha_{k+p}\right]\left[J_q - J_{p-q}\right],\\ \Gamma^{(4)}_{k,p,q} &= -4J'_p\left[\alpha_k - \alpha_{k+p}\right]\left[J_q - J_{k+p-q}\right],\\ \Gamma^{(5)}_{k,p,q} &= -J'_qJ'_p\left[J_k - J_{k+p}\right],\\ \Gamma^{(6)}_{k,p,q} &= -J'_qJ'_p\left[\alpha_k - \alpha_{k+p}\right]. \quad (A4)\end{aligned}$$

The commutator $[\eta_2, H_1]$ is obtained from $[\eta_1, H_1]$ by replacing $\Gamma^{(5)}$ by $\Gamma^{(6)}$ and interchanging $S^\alpha \leftrightarrow \sigma^\alpha$.

APPENDIX B: BOSONIZATION

In order to bosonize the Hamiltonian (15) it is convenient to tranform the spin operators to coordinate space. At weak coupling the generated interactions are short-ranged. In a continuum description the most relevant (in the renormalization group sense) contributions can then be obtained by considering nearest-neighbour terms. Interactions between next nearest neighbours will merely lead to a renormalization of the couplings as well as generate (less relevant) derivative terms. Using (10) and keeping only the terms corresponding to nearest-neighbour interactions we find

$$\begin{aligned}H(l) \sim\ & J(l)\sum_i\mathbf{S}(i)\cdot\mathbf{S}(i+1) + \alpha(l)\sum_i\boldsymbol{\sigma}(i)\cdot\boldsymbol{\sigma}(i+1)\\ +\ & J'(l)\sum_i\mathbf{S}(i)\cdot\boldsymbol{\sigma}(i) + \widetilde{J}'(l)\sum_i\mathbf{S}(i)\cdot(\boldsymbol{\sigma}(i+1)+\boldsymbol{\sigma}(i-1))\\ +\ & M^{(1)}(l)\sum_i\mathbf{S}(i)\cdot\boldsymbol{\sigma}(i+1)\ \mathbf{S}(i+1)\cdot\boldsymbol{\sigma}(i) + M^{(2)}(l)\sum_i\mathbf{S}(i)\cdot\mathbf{S}(i+1)\ \mathbf{S}(i-1)\cdot(\boldsymbol{\sigma}(i)-\boldsymbol{\sigma}(i+1))\\ +\ & M^{(3)}(l)\sum_i\mathbf{S}(i)\cdot\mathbf{S}(i+1)\ \boldsymbol{\sigma}(i)\cdot\boldsymbol{\sigma}(i+1) + M^{(4)}(l)\sum_i\boldsymbol{\sigma}(i)\cdot\boldsymbol{\sigma}(i+1)\ \boldsymbol{\sigma}(i-1)\cdot(\mathbf{S}(i)-\mathbf{S}(i+1))\\ +\ & iM^{(5)}(l)\sum_i[\mathbf{S}(i)\times\mathbf{S}(i+1)]\cdot(\boldsymbol{\sigma}(i)-\boldsymbol{\sigma}(i+1)) + iM^{(6)}(l)\sum_i[\boldsymbol{\sigma}(i)\times\boldsymbol{\sigma}(i+1)]\cdot(\mathbf{S}(i)-\mathbf{S}(i+1)). \quad (B1)\end{aligned}$$

We now bosonize the part $H_0 = J(l)\sum_i\mathbf{S}(i)\cdot\mathbf{S}(i+1)$ of the Hamiltonian (B1) by standard methods, see e.g.,[33,41,42,43,44]

$$S^\alpha(j) \simeq J^\alpha(z) + \bar{J}^\alpha(\bar{z}) + (-1)^j n^\alpha(x)\ , \quad (B2)$$

$$\begin{aligned}J^+(z) &= \frac{a_0}{2\pi}e^{-i\varphi(z)}\ , \qquad \bar{J}^+(\bar{z}) = \frac{a_0}{2\pi}e^{i\bar{\varphi}(z)}\ ,\\ J^z(z) &= -i\frac{a_0}{4\pi}\partial_z\varphi\ , \qquad \bar{J}^z(\bar{z}) = -\frac{a_0}{4\pi}\partial_{\bar{z}}\bar{\varphi}\ ,\\ \mathbf{n}(x) &= c\sqrt{a_0}\Big(\cos(\frac{\Theta}{2}), -\sin(\frac{\Theta}{2}), -\sin(\frac{\Phi}{2})\Big). \quad (B3)\end{aligned}$$

Here $z = v\tau - ix$, $\bar{z} = v\tau + ix$, $\Phi = \varphi + \bar{\varphi}$, $\Theta = \varphi - \bar{\varphi}$ and we use a normalization such that

$$\left\langle e^{i\alpha\varphi(z)}e^{-i\alpha\varphi(0)}\right\rangle = z^{-2\alpha^2}\ . \quad (B4)$$

The bosonized form of H_0 is

$$H_0 = \frac{v_s(l)}{16\pi}\int dx[(\partial_x\Phi)^2 + (\partial_x\Theta)^2]. \quad (B5)$$

Using operator product expansions we then can extract the dominant parts of the various other terms in (B1). Denoting $x = ja_0$ we have

$$\mathbf{S}(j)\cdot\mathbf{S}(j+1)\boldsymbol{\sigma}(j)\cdot\boldsymbol{\sigma}(j+1) \sim \Big[c_1+(-1)^j c_2\cos\big(\frac{\Phi}{2}\big)\Big]\boldsymbol{\sigma}(j)\cdot\boldsymbol{\sigma}(j+1)+\ldots, \tag{B6}$$

$$\mathbf{S}(j)\cdot\boldsymbol{\sigma}(j+1)\ \mathbf{S}(j+1)\cdot\boldsymbol{\sigma}(j) \sim \Big[c_1+(-1)^j c_2\cos\big(\frac{\Phi}{2}\big)\Big]\boldsymbol{\sigma}(j)\cdot\boldsymbol{\sigma}(j+1)+c_3[\mathbf{J}(x)-\bar{\mathbf{J}}(x)]\cdot\boldsymbol{\sigma}(j)+\ldots, \tag{B7}$$

$$\big(\mathbf{S}(j)\times\mathbf{S}(j+1)\big)\cdot\boldsymbol{\sigma}(j) \sim 2c_3\ [\mathbf{J}(x)-\bar{\mathbf{J}}(x)]\cdot\boldsymbol{\sigma}(j)+\ldots, \tag{B8}$$

$$\mathbf{S}(j)\cdot\mathbf{S}(j+1)\mathbf{S}(j-1)\cdot\boldsymbol{\sigma}(j)-\mathbf{S}(j-1)\cdot\mathbf{S}(j)\mathbf{S}(j-2)\cdot\boldsymbol{\sigma}(j)\propto(-1)^j\mathbf{n}(x)\cdot\boldsymbol{\sigma}(j). \tag{B9}$$

As expected, the interactions generated under the flow are simply all terms that are compatible with the global spin rotational $SU(2)$ symmetry. The term $(\mathbf{J}(x)-\bar{\mathbf{J}}(x))\cdot\boldsymbol{\sigma}(j)$ breaks the left-right (chiral) symmetry of the free boson Hamiltonian in the $J'\to 0$ limit. However, it is well known[45] that interchange of left and right moving bosons is not a symmetry of the spin-1/2 Heisenberg model at low energies due to the presence of a marginally irrelevant interaction of spin currents (which we have omitted in (B5) for the sake of brevity). Inspection of the scaling dimensions of the bosonic parts of the various terms generated along the flow suggests that at low energies the most relevant interaction of staggered magnetizations is precisely the one picked out by our decoupling scheme (18). We note that the term (B8) is not included in our decoupling scheme. While it is likely to be as relevant as $\boldsymbol{\mathcal{J}}\cdot\boldsymbol{\sigma}$, the bare coupling of the latter is much larger, which justifies neglecting the former in the weak coupling regime $J'\ll J$.

Another fluctuation induced contribution that is not included in our decoupling scheme is the interation of dimerizations

$$(-1)^j\cos\big(\frac{\Phi(x)}{2}\big)\ \boldsymbol{\sigma}(j)\cdot\boldsymbol{\sigma}(j+1). \tag{B10}$$

It is less relevant than the terms we keep. If it were the dominant interaction in the problem, its effect would be to open up dimerization gaps among the Kondo spins and spin-chain spins respectively.

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